

On The Existence of Roton Excitations in Bose Einstein Condensates: Signature of Proximity to a Mott Insulating Phase

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Within the last decade, artificially engineered Bose Einstein Condensation has been achieved in atomic systems. Bose Einstein Condensates are superfluids just like bosonic Helium is and all interacting bosonic fluids are expected to be at low enough temperatures. One difference between the two systems is that superfluid Helium exhibits roton excitations while Bose Einstein Condensates have never been observed to have such excitations. The reason for the roton minimum in Helium is its proximity to a solid phase. The roton minimum is a consequence of enhanced density fluctuations at the reciprocal lattice vector of the stillborn solid. Bose Einstein Condensates in atomic traps are not near a solid phase and therefore do not exhibit roton minimum. We conclude that if Bose Einstein Condensates in an optical lattice are tuned near a transition to a Mott insulating phase, a roton minimum will develop at a reciprocal lattice vector of the lattice. Equivalently, a peak in the structure factor will appear at such a wavevector. The smallness of the roton gap or the largeness of the structure factor peak are experimental signatures of the proximity to the Mott transition.

In the present work we focus attention in the possible existence or nonexistence of roton excitations in artificially engineered Bose Einstein Condensates (BECs)[1, 2, 3]. BECs are superfluid as they possess a finite sound speed[4, 5, 6] and reduced long wavelength scattering[7, 8]. The other important bosonic superfluid is He₄[5, 9]. Since BECs and He₄ are the same universal phase of matter, they share a large commonality. For example, they are both superfluids whose elementary long wavelength excitation spectrum is phononic, their ground states spontaneously break gauge invariance[10], that is their ground states exhibit macroscopic quantum coherence, and they both possess vortex excitations[11]. This is an example of universality of stable fixed points of matter. In these cases the superfluid ground state is such a fixed point. The similarities will become ever more apparent as the low energy properties BECs are studied more carefully.

On the other hand, at shorter wavelengths Helium possesses a roton minimum[5, 6, 12] in its excitation spectrum leading to low energy excitations occurring at a specific wavevector, which are gapped and are different than long wavelength sound. These excitations can make important contributions to the dynamics and thermodynamics of the system. In BECs no such excitation has been observed and the lack of a peak in the structure factor[7] leads to the conclusion that they do not possess roton excitations. We review some of the properties of rotons in Helium and determine under what conditions will they occur in BECs.

All quantum many particle systems are described by a Hamiltonian[5]

$$\mathcal{H} = \int \left(m \frac{\vec{v} \cdot \rho \vec{v}}{2} \right) d^3r + U[\rho] \quad (1)$$

where $m\vec{v} \cdot \rho \vec{v}/2$ is the kinetic energy operator, $U[\rho]$ is the potential energy operator, which in general can be a

functional of the density operator. The density operator in first quantized notation is

$$\rho(\vec{r}) = \sum_i \delta(\vec{r} - \vec{r}_i) \quad (2)$$

with \vec{r}_i being the position of the i th particle. The velocity operator is in first quantized notation

$$\vec{v}(\vec{r}) = \sum_i \left[\frac{\vec{p}}{2m} \delta(\vec{r} - \vec{r}_i) + \delta(\vec{r} - \vec{r}_i) \frac{\vec{p}}{2m} \right] \quad (3)$$

with commutation relations

$$[\rho(\vec{r}'), \vec{v}(\vec{r})] = i \frac{\hbar}{m} \nabla \delta(\vec{r}' - \vec{r}) \quad (4)$$

The ground state of the Hamiltonian (1) could be a quantum fluid or solid depending on the interaction. We will suppose it to be a fluid as we have BECs and Helium in mind.

We study the excitation spectrum of the bosonic fluid on quite general grounds following Landau[5] and the Russian school[13] quite closely. We suppose the density to have a well defined average which we take to be uniform for simplicity. This will not change the nature of the considerations, although in real life the density can be modulated by the lattice as for BECs in optical lattices. The average velocity is zero as we consider a system at rest. We Fourier expand the density and velocity operators about their averages:

$$\rho(\vec{r}) = \rho_0 + \frac{1}{N} \sum_{\vec{k}} \rho_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} \quad (5)$$

$$\vec{v}(\vec{r}) = \frac{1}{N} \sum_{\vec{k}} v_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} \quad (6)$$

where we are using the lattice normalization, the number of sites N instead of the volume V . Quantum mechanically, the velocity is proportional to the gradient of the

local phase variable of the particle, $\vec{v}(\vec{r}) = \hbar/m\nabla\theta$, or in Fourier components

$$\vec{v}_{\vec{k}} = \frac{i\hbar\vec{k}}{m}\theta_{\vec{k}} \quad (7)$$

The density velocity commutation relation (4) imply the well known density phase commutation relation

$$[\rho_{\vec{k}}, \theta_{-\vec{k}'}] = i\delta_{\vec{k}\vec{k}'} \quad (8)$$

i.e. $\hbar\theta_{-\vec{k}}$ is the momentum conjugate to the density fluctuation $\rho_{\vec{k}}$. The Hamiltonian (1) thus becomes

$$\mathcal{H} = U(\rho_0) + \frac{1}{N} \sum_{\vec{k}} \left\{ \frac{\rho_0 \hbar^2 k^2}{2m} |\theta_{-\vec{k}}|^2 + \frac{1}{2} \left(U_{\vec{k}} + \frac{\hbar^2 k^2}{4m\rho_0} \right) |\rho_{\vec{k}}|^2 \right\} \quad (9)$$

where $U_{\vec{k}}$ is the Fourier transform of the interaction. The interaction is completely general. The only requirements are that $U_{\vec{k}=0}$ is a constant, so that we can have a superfluid, and that there is some short range repulsion analogous to a Hubbard term that can be turned up in order to stabilize a Mott insulating phase. $(\hbar^2 k^2)/(4m\rho_0)|\rho_{\vec{k}}|^2$ is the elastic energy associated with changing the density. This last term comes from acting the Hamiltonian on the wavefunction and making sure that one keeps careful track of both density and phase degrees of freedom[14] in the full quantum mechanical kinetic energy term. We have performed studies very near to these in the context of fermionic systems[15] which we follow very closely in the present note. Charged boson systems were studied previously[14] with the Quantum Hall effect in mind.

The quantum liquid is thus a collection of harmonic oscillators in momentum space for the density fluctuations. The mass and spring constant of the oscillators are

$$M_{\vec{k}} \equiv \frac{m}{\rho_0 k^2}, \quad K_{\vec{k}} \equiv U_{\vec{k}} + \frac{\hbar^2 k^2}{4m\rho_0}. \quad (10)$$

The density energy excitation spectrum of the quantum liquid is

$$E_{\vec{k}} = \hbar\omega_{\vec{k}}(n + 1/2) \quad (11)$$

$$\omega_{\vec{k}}^2 = \frac{K_{\vec{k}}}{M_{\vec{k}}} = \frac{\rho_0 k^2}{m} \left(U_{\vec{k}} + \frac{\hbar^2 k^2}{4m\rho_0} \right) \quad (12)$$

The ground state energy is given by $U(\rho_0) + \sum_{\vec{k}} \hbar\omega_{\vec{k}}/2$. We note that the Virial theorem implies that

$$\frac{1}{2} \hbar\omega_{\vec{k}} N = \left(U_{\vec{k}} + \frac{\hbar^2 k^2}{4m\rho_0} \right) \langle |\rho_{\vec{k}}|^2 \rangle$$

$$\hbar\omega_{\vec{k}} = \frac{\hbar^2 k^2}{2mS(\vec{k})} \quad (13)$$

where the structure factor is defined by

$$S(\vec{k}) = \frac{\langle |\rho_{\vec{k}}|^2 \rangle}{N\rho_0} \quad (14)$$

which is, of course, the Fourier transform of the density-density correlation function. For the quantum liquid we thus have

$$S(\vec{k}) = \frac{\hbar k}{2m} \frac{1}{\sqrt{\frac{\rho_0}{m} \left(U_{\vec{k}} + \frac{\hbar^2 k^2}{4m\rho_0} \right)}} \quad (15)$$

The ground state energy will have the density oscillators unexcited. Hence, if the ground state wavefunction of the bosonic system *without density correlations* is $|\psi_{GS}\rangle$, the ground state wavefunction *with density correlations* is

$$|\psi\rangle = \exp \left\{ -\frac{1}{2} \sum_{\vec{k}} \sqrt{\frac{m}{\rho_0 \hbar^2 k^2} \left(U_{\vec{k}} + \frac{\hbar^2 k^2}{4m\rho_0} \right)} |\rho_{\vec{k}}|^2 \right\} |\psi_{GS}\rangle. \quad (16)$$

The factor in front appears because it is the ground state wavefunction of harmonic oscillators and the minimum energy condition is obviously to have the oscillators shaking as little as possible. We see that the factor suppresses density fluctuations. The wavefunction is essentially exact to quadratic order in the density fluctuations.

Since the Hamiltonian and ground state wavefunction do not contain any periodic lattice effects, they aptly describe systems with no external lattice such as liquid Helium, to which we turn our discussion now. The ground state wavefunction (16) does not contain any insulating crystalline order as $\langle \rho_{\vec{k}} \rangle = 0$ for all \vec{k} . When the system spontaneously solidifies, it will exhibit Bragg peaks at the reciprocal lattice vectors, \vec{Q} , corresponding to the insulating crystal. These peaks mean that $\langle \rho_{\vec{Q}} \rangle \neq 0$. We inquire into the behavior when the boson fluid approaches a solidification transition.

Proximity to a solid phase with reciprocal lattice vector \vec{Q} for the incipient order softens the spring constant of the density oscillators of the liquid, $K_{\vec{Q}} \rightarrow 0$, which makes $\omega_{\vec{Q}} \rightarrow 0$. This last condition means the mode becomes degenerate with the ground state and there will be enhanced density fluctuations, $\langle |\rho_{\vec{Q}}|^2 \rangle \rightarrow \infty$ at the wavevector of the stillborn solid, i.e. the system is approaching a phase transition. The diverging fluctuations follow because the position fluctuations of a harmonic oscillator diverge as the spring constant vanishes due to the Heisenberg uncertainty principle. The softening of the density mode implies that the interaction $U_{\vec{k}}$ has a minimum at \vec{Q} which in turn produces a peak in the structure factor, $S(\vec{Q})$, that diverges as one approaches the point when the system solidifies. This peak in the structure factor implies will drag the spectrum down according to the equation (13) creating a roton minimum[12].

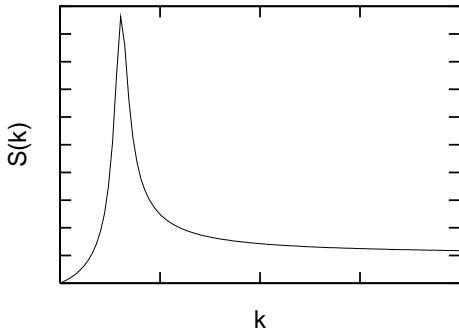


FIG. 1: Structure factor vs. wavevector for a Bose fluid near a solidification transition. The density fluctuation peak at the wavevector of the incipient order is clearly visible.

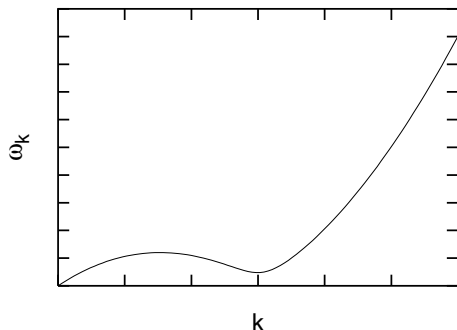


FIG. 2: Frequency dispersion for a Bose fluid near a solidification transition. The roton minimum at the wavevector of the incipient order is clearly visible.

We thus have as a simple phenomenological model that captures the physics

$$U_{\vec{k}} = \frac{U}{k^2 + k_0^2} - \frac{U}{Q^2 + k_0^2} + \alpha \frac{\hbar^2}{4m\rho_0} (\vec{k} - \vec{Q})^2 - \alpha \frac{\hbar^2 k^2}{4m\rho_0} + \Delta$$

where k_0 is some microscopic scale that characterizes the interaction, nonzero α makes a roton minimum, and $\Delta - \alpha \frac{\hbar^2 Q^2}{4m\rho_0}$ is the roton gap, which will collapse at the crystallization transition as the smallness of the gap of such a roton is a measure of proximity to crystallization. The first term in the potential represents the short range repulsion, chosen for simplicity to have a Yukawa form. The parameter Δ can be thought of as the long range repulsion. From the form of the interaction we get the structure factor and the density excitation spectrum for Helium, which we plot in Figures 1 and 2. We emphasize that the reason for the roton minimum in the excitation spectrum is the proximity of the liquid Helium ground state to a solid phase. Helium is an almost solid barely melted by quantum fluctuations, i.e. it is a very strongly correlated liquid.

We now turn our attention to BECs in optical lattices. These superfluids do not exhibit roton minimum in their excitation spectrum. The reason for this is that unless

the wells of the optical lattice are made deep, the system is far from a solid or Mott insulating phase. In fact, it is an extremely good approximation to take the interaction potential to be a constant $U_{\vec{k}} = I$. For such a case, we plot in Figures 3 and 4 the structure factor and density excitation spectrum. We see no peak in the structure factor or roton minimum in the excitation spectrum as observed experimentally[7].

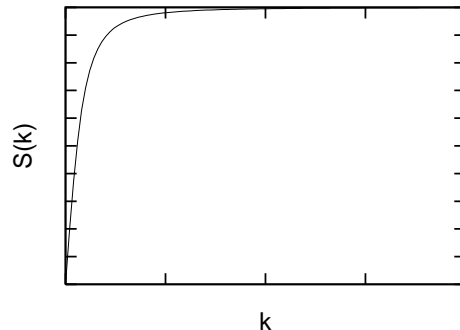


FIG. 3: Structure factor vs. wavevector for a Bose fluid far from a solidification transition. There is no peak.

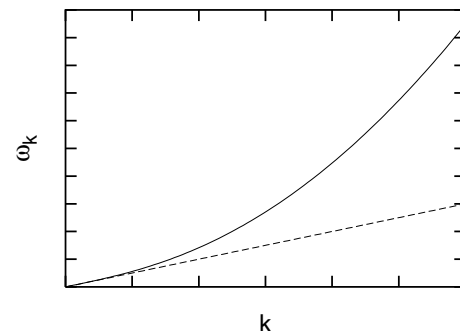


FIG. 4: Frequency dispersion for a Bose fluid far from a solidification transition. The upper graph is the superfluid dispersion and the lower one is a phononic linear dispersion in order to make apparent the linearity of the superfluid dispersion at long wavelengths. There is no roton minimum.

So far we have neglected optical lattice effects because even though they make quantitative changes to measurable parameters of the BEC superfluid, they do not change the universal superfluid physics. On the other hand, as one approaches a commensurate Mott insulating phase, the lattice will become ever more important. The presence of the optical lattice implies that there is an external potential $-V_{\vec{k}}$ that acts on the bosons thus adding to the Hamiltonian (9) the term

$$\mathcal{H}_{\text{ext}} = - \sum_{\vec{k}} V_{\vec{k}} \rho_{\vec{k}}. \quad (17)$$

The effect of the extra term in the ground state wavefunction is to move the equilibrium position of the density

oscillators from $\langle \rho_{\vec{k}} \rangle = 0$ to

$$\langle \rho_{\vec{k}} \rangle = \frac{V_{\vec{k}}}{U_{\vec{k}} + \frac{\hbar^2 k^2}{4m\rho_0}}. \quad (18)$$

The fact that there is $\langle \rho_{\vec{k}} \rangle \neq 0$ *does not* mean the boson fluid *in an optical lattice* has solidified into an insulating phase. It just means that the boson fluid is being modulated by the periodic lattice. It is true that in the insulating phase this expected value will be nonzero too. If there was not an external lattice, $\rho_{\vec{k}} \neq 0$ for some \vec{k} 's would imply an insulating phase as the only way this can happen is for the system to spontaneously break translational invariance. So the question of how to determine if one is in the Mott phase is delicate for lattice boson systems.

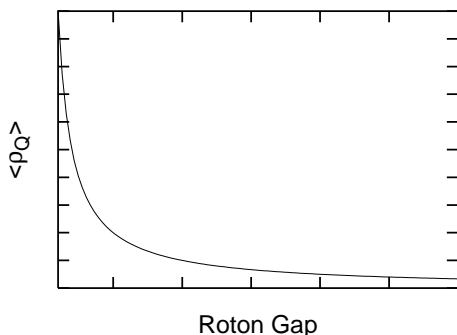


FIG. 5: Density Fourier component at the wavevector of the incipient order vs. roton gap for a Bose fluid near a solidification transition. The divergence as the roton gap goes to zero is a signature of the imminent transition.

A way to know that the bosons in an optical lattice have solidified into a commensurate Mott phase is to look at the density excitation spectrum or the structure factor. When it has solidified, the excitation spectrum will have a gap at long wavelengths and the structure factor will go like k^2 at long wavelengths. This is not a violation of Goldstone's theorem[16] as the lattice was not generated spontaneously by the boson system but is provided by the external lattice potential, i.e. the symmetry is explicitly broken. Our interest is what are the signatures of the incipient Mott insulating phase. As mentioned above, one can know the transition is approaching by a softening of the excitation spectrum at appropriate wavevectors. In this case, the system will behave exactly as Helium, exhibiting roton minimum and its structure factor and energy excitation spectrum will be as shown in Figures 1 and 2. Moreover, from the formula for the response of the lattice potential (18), we see that the density Fourier component at the roton wavevector will grow as the roton gap collapses. We plot the growth of such a Fourier component vs. size of the roton gap in Figure 5.

Summarizing, artificially engineered BECs and liquid He_4 are both quantum bosonic superfluids. They share

a large similarity of intrinsically quantum behavior for their ground states and low energy states. One important difference is that Helium possesses roton excitations while BECs appear not to have them. The reason for this is that BECs in the atomic traps are far from being a solid. Helium possesses a roton because it is a stillborn solid where quantum fluctuations barely prevent solidification.

On the other hand, BECs in optical lattices[17, 18, 19] can be tuned near a solidification or Mott transition by making the wells deeper. We thus predict that near a transition from a superfluid BEC to a commensurate Mott phase in an optical lattice there will be roton excitations measurable by light scattering occurring at the reciprocal lattice vector of the lattice. Their experimental signatures will be a large peak in the structure factor or a roton minimum in the excitation spectrum. The smallness of the roton gap or height of the structure factor peak can be used as diagnostics of the proximity to the incipient Mott order. The roton excitation adds to the list of intrinsically quantum mechanical excitations that exists in BECs and will be of importance to the dynamics of the systems.

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- [1] K. B. Davis *et. al.*, Phys. Rev. Lett. **75**, 3969 (1995).
 - [2] C. C. Bradley *et. al.*, Phys. Rev. Lett. **75**, 1687 (1995).
 - [3] M. H. Anderson *et. al.*, Science **269**, 198 (1995).
 - [4] M. R. Andrews *et. al.*, Phys. Rev. Lett. **79**, 553 (1997).
 - [5] L. D. Landau, Journal of Physics **V**, 71-90 (1941).
 - [6] N. N. Bogolyubov, J. Phys. USSR **11**, 23 (1947).
 - [7] W. Ketterle *et. al.*, Phys. Rev. Lett. **83**, 2876 (1999).
 - [8] A. Görlitz *et. al.*, Phys. Rev. A **63**, 041601 (2001).
 - [9] P. Nozières and D. Pines, *The Theory of Quantum Liquids*, Perseus Books (1966).
 - [10] P. W. Anderson, Rev. Mod. Phys. **38**, 298 (1966).
 - [11] M. R. Matthews *et. al.*, Phys. Rev. Lett. **83**, 2498 (1999).
 - [12] R. P. Feynman, Phys. Rev. **94**, 262 (1954); R. P. Feynman and M. Cohen, Phys. Rev. **102**, 1189 (1956).
 - [13] A. A. Abrikosov *et. al.*, "Methods of Quantum Field Theory in Statistical Physics", Prentice Hall, Englewood Cliffs, NJ (1963).
 - [14] C. Kane *et. al.*, Phys. Rev. B **43**, 3255 (1991).
 - [15] Z. Nazario and D. I. Santiago, e-print arXiv: cond-mat/0403374 (2004).
 - [16] J. Goldstone, Nuovo cimento **19**, 154 (1961); J. Goldstone *et. al.*, Phys. Rev. **127**, 965-970 (1962).
 - [17] M. Greiner *et. al.*, Nature **415**, 39 (2002).
 - [18] M.P.A. Fisher *et al*, Phys. Rev. B. **40**, 546 (1989)
 - [19] Z. Nazario and D. I. Santiago, e-print arXiv: cond-mat/0308005 (2003).